

Supplementary data for the article:

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# Mono- and binuclear Ru(II) arene complexes with (fluoro substituted) picolinic acid: synthesis, characterization and cytotoxicity

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## Supporting Information

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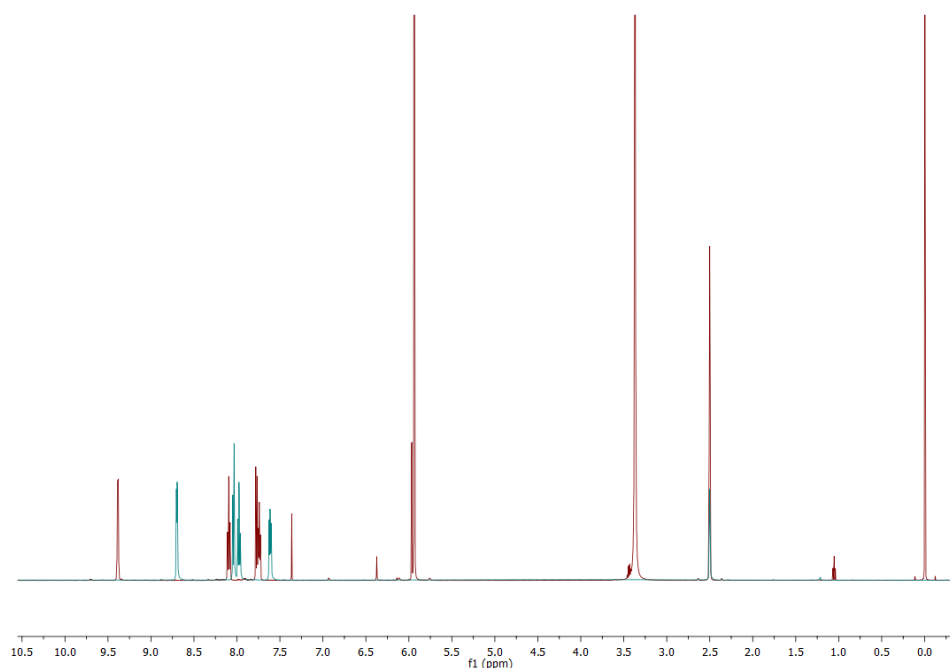
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<sup>1</sup>H NMR spectra of **1** and **5** ..... S9–10

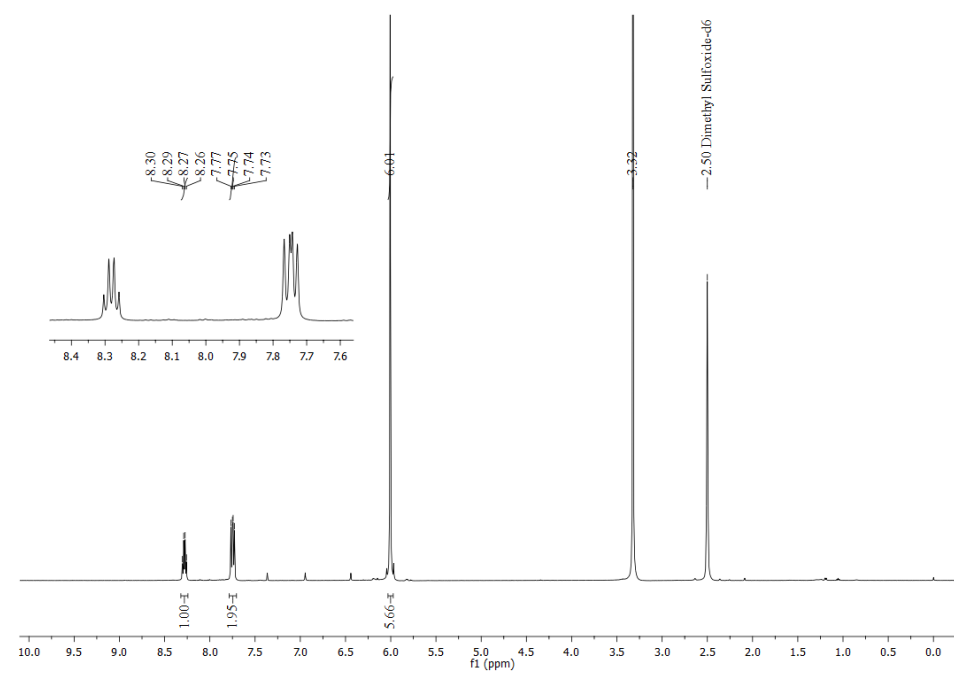
#### SM.3. Cytotoxicity analysis- Selectivity Index determination

TS1. Selectivity Index (SI) for **1–8** and cisplatin

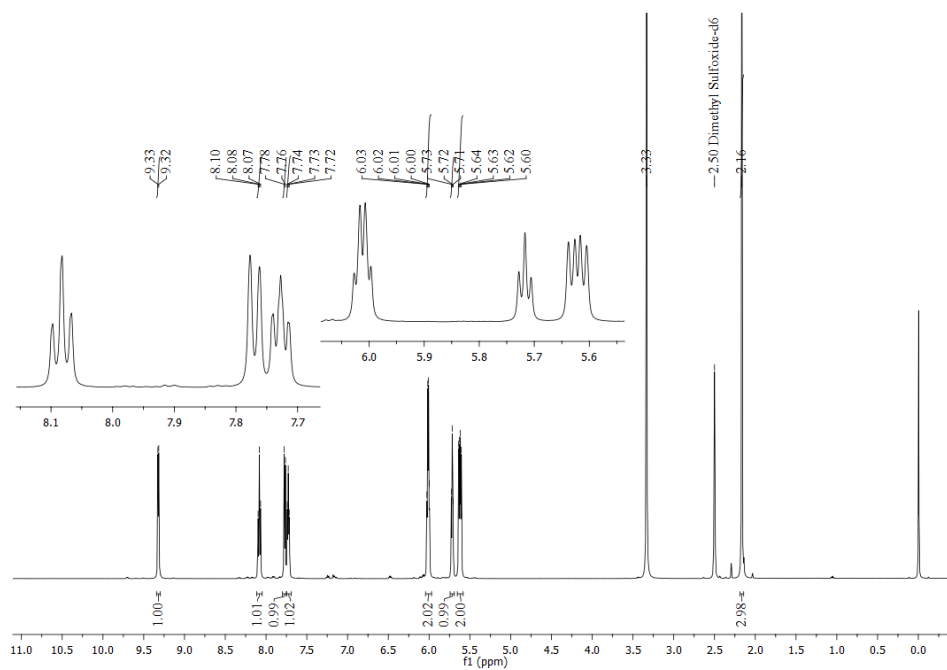
### SM.1. NMR Spectroscopy



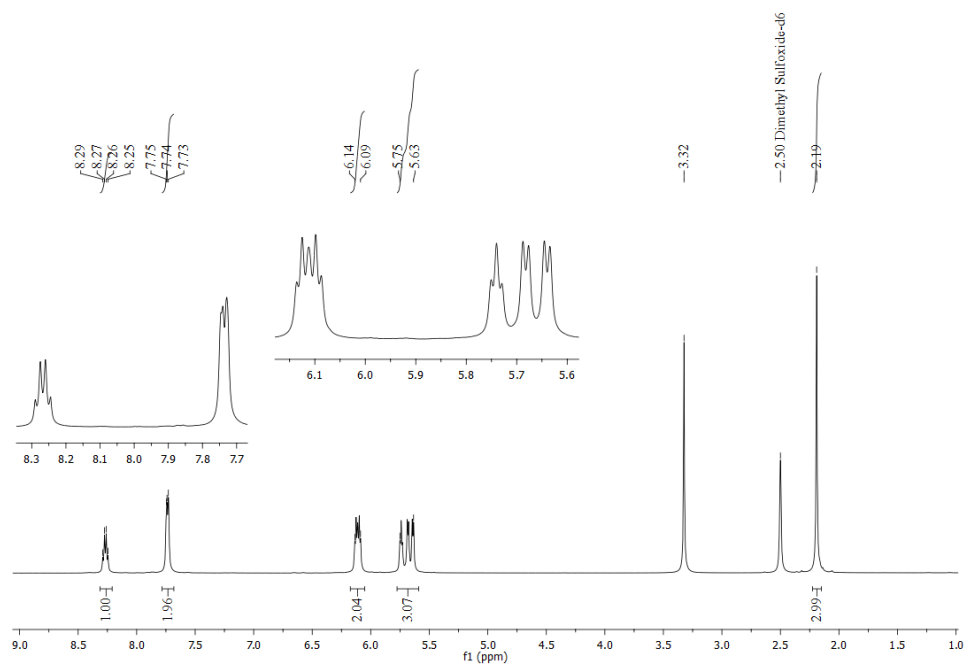
**Figure S1:** <sup>1</sup>H NMR spectra of **1** (red line) overlapped with the ligand, picolinic acid, (green line) recorded in DMSO.



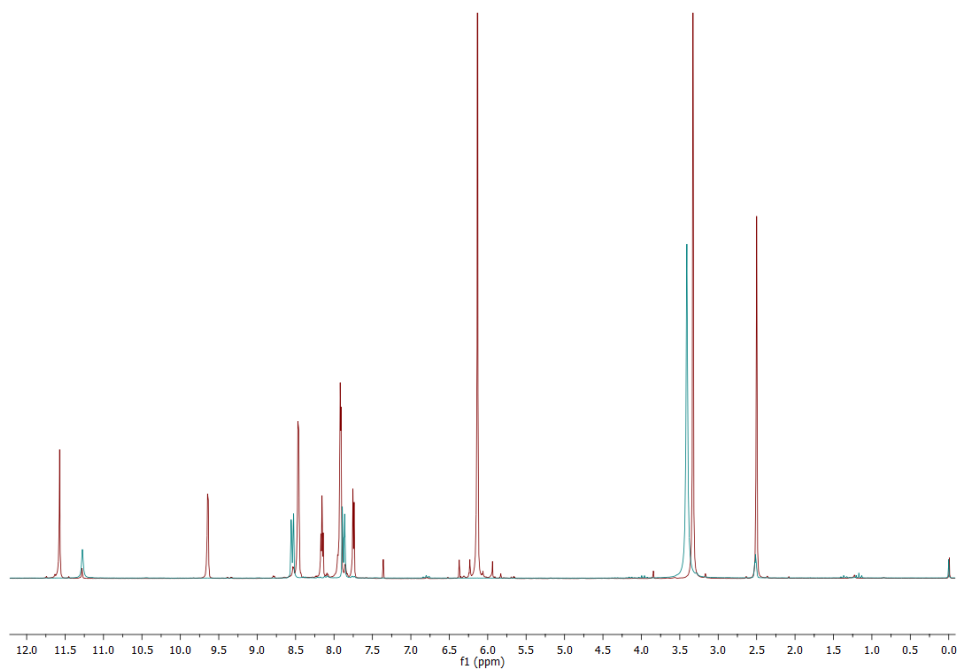
**Figure S2:** <sup>1</sup>H NMR spectrum of **2** recorded in DMSO.



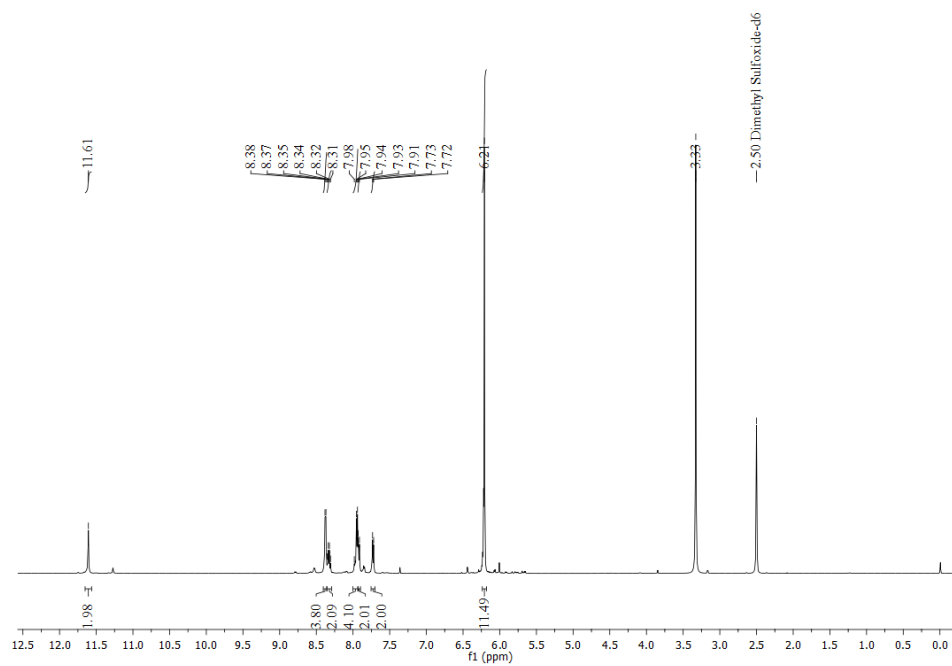
**Figure S3:** <sup>1</sup>H NMR spectrum of **3** recorded in DMSO.



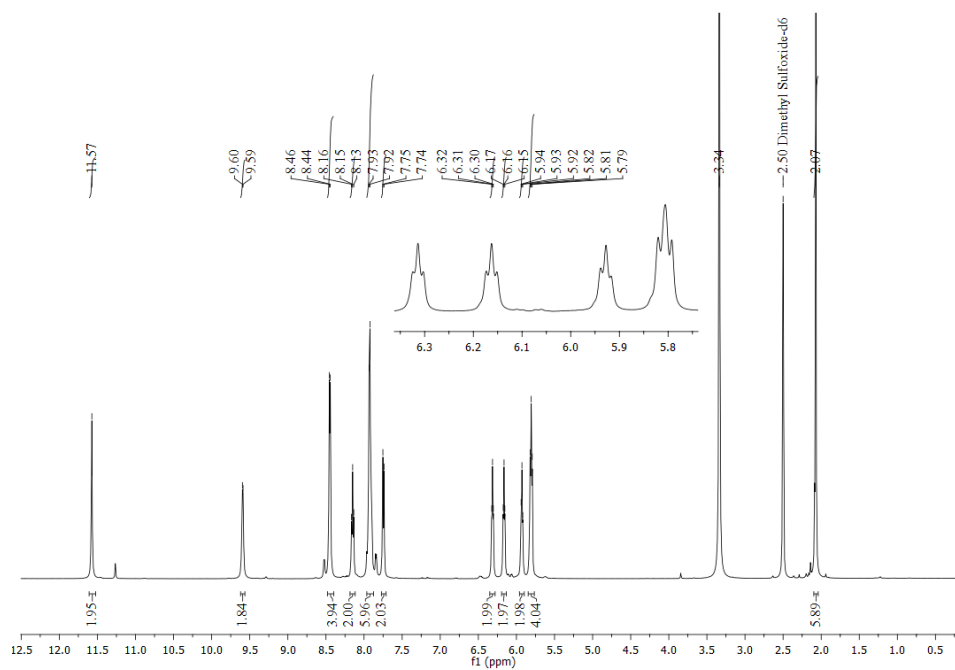
**Figure S4:** <sup>1</sup>H NMR spectrum of **4** recorded in DMSO.



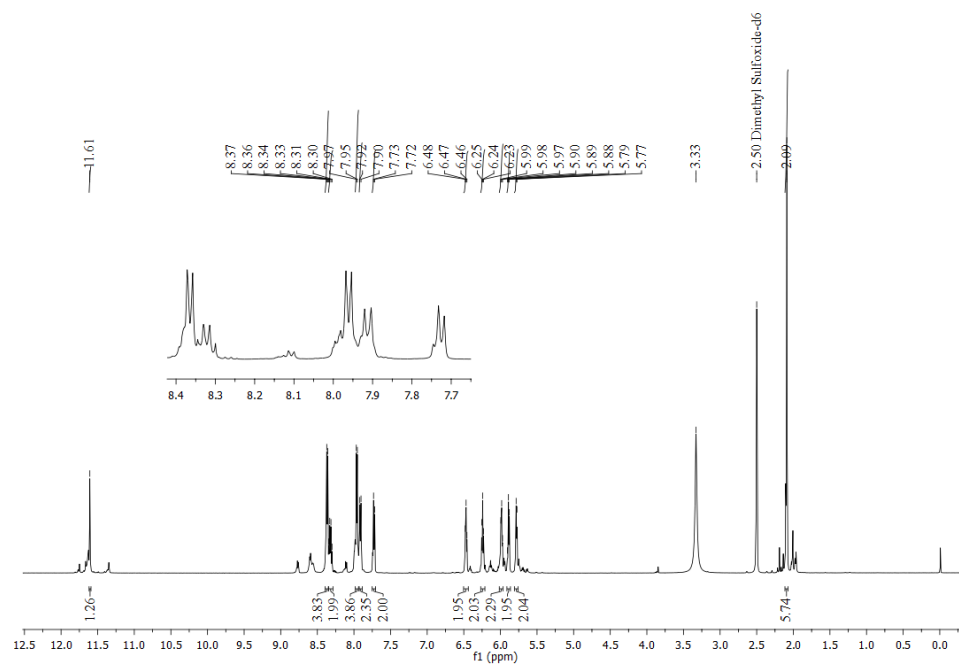
**Figure S5:** <sup>1</sup>H NMR spectra of **5** (red line) overlapped with the ligand, *N,N'*-di(4-pyridinyl)ethanediamide, (green line) recorded in DMSO.



**Figure S6:**  $^1\text{H}$  NMR spectrum of **6** recorded in DMSO.

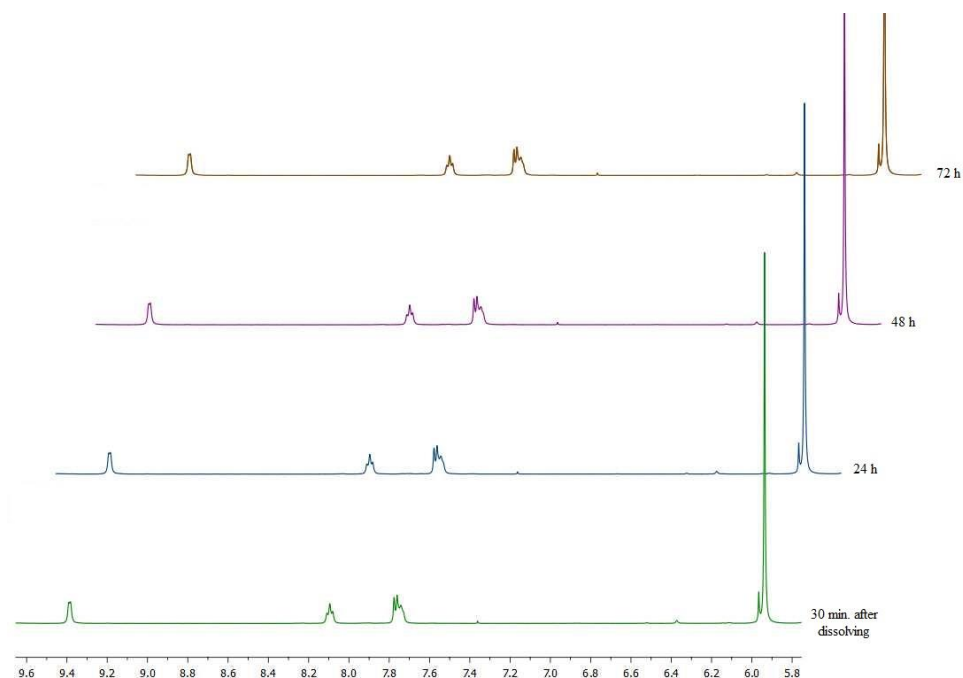


**Figure S7:**  $^1\text{H}$  NMR spectrum of **7** recorded in DMSO.

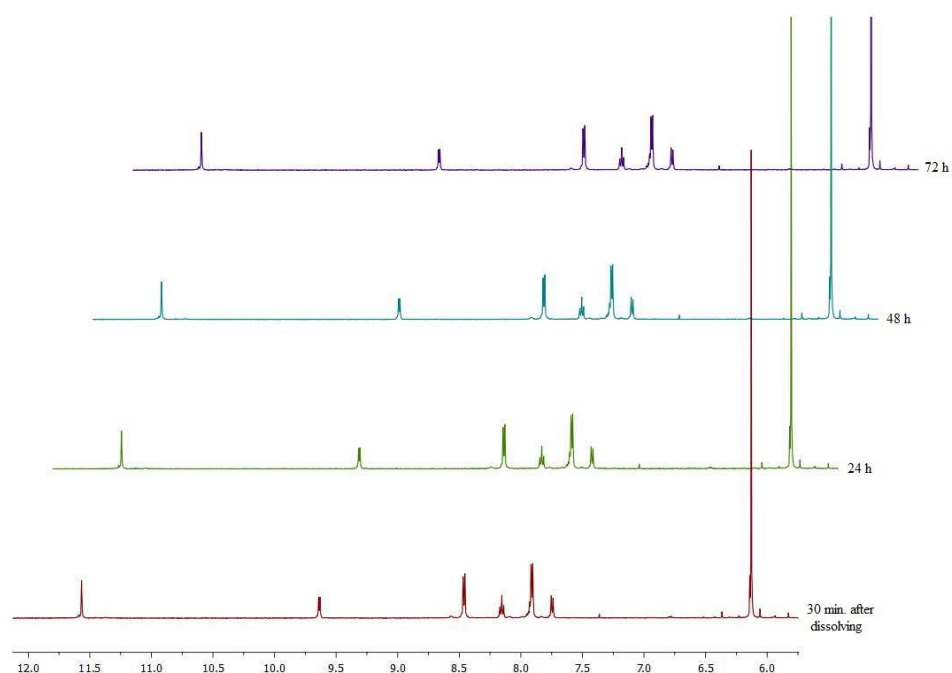


**Figure S8:**  $^1\text{H}$  NMR spectrum of **8** recorded in DMSO.

## SM.2. Chemical behavior of the Ru(II)-arenes in DMSO



**Figure S9:**  $^1\text{H}$  NMR comparative spectra of **1** in DMSO as a function of time (0, 24, 48, and 72 h).



**Figure S10:**  $^1\text{H}$  NMR comparative spectra of **5** in DMSO as a function of time (0, 24, 48, and 72 h).

### SM.3. Cytotoxicity analysis- Selectivity Index determination

**Table TS1.** Table shows the values of the Selectivity Index (SI), for **1-8** and cisplatin, calculated as the ratio between  $\text{IC}_{50}$  ( $\mu\text{M}$ ) obtained for normal fibroblast cells (MRC-5), and those  $\text{IC}_{50}$  ( $\mu\text{M}$ ) values obtained in tumor cells.

SI - Selectivity index								
Compound	$\text{SI}_{\text{A549}}$	$\text{SI}_{\text{HTB177}}$	$\text{SI}_{\text{PC3}}$	$\text{SI}_{\text{A375}}$	$\text{SI}_{\text{HeLa}}$	$\text{SI}_{\text{HCT116}}$	$\text{SI}_{\text{MDA453}}$	$\text{SI}_{\text{A549}}$
<b>1</b>	0.3	0.3	0.3	0.5	1.1	1.5	0.6	0.3
<b>2</b>	/*	/	/	0.7	1.1	0.7	0.8	/
<b>3</b>	0.3	0.4	0.2	0.3	0.7	0.6	0.4	0.3
<b>4</b>	/	/	/	/	1.0	0.7	0.7	/
<b>5</b>	0.3	0.3	0.3	0.3	0.7	0.5	0.6	0.3
<b>6</b>	0.4	/	0.4	0.4	0.8	0.5	0.6	0.4
<b>7</b>	0.5	0.4	0.3	0.4	0.8	0.6	0.6	0.5
<b>8</b>	0.5	0.4	0.5	0.5	0.8	0.4	0.7	0.5
<b>Cisplatin</b>	0.3	0.3	0.3	0.5	1.1	1.5	0.6	0.3

\* SI was not determined, as  $\text{IC}_{50}$  ranging above 300 ( $\mu\text{M}$ ).